

第1講 群論再考(最高！)

-点群を中心に-

分類 点群が決定されると

→ 分子構造 分子軌道 振動モード 結合様式などの分子の性質がすべて影響を受ける

直感的分類のスズメ σ は鏡映面、 n は $(360/n)^\circ$ の回転 $()$ は対応イメージ

1 対称性少なそう? C_1 (なし) C_s (面对称= S_1) C_i (点对称= S_2)

2 多面体 T_d (4面体) O_h (8面体) I_h (12面体) D_{2h} (直方体)

3 直線 $C_{\infty v}$ (円錐、両端が違う) $D_{\infty h}$ (円柱、両端が同じ)

4 非直線 C_{nv} (正 n 角錐、 $C_n + \sigma_v$)

D_{nh} (正 n 角柱、歯車、 $C_n + \sigma_h + \sigma_v$)

C_n (プロペラ C_{nv} にヒゲがついている)

C_{nh} ($C_n + \sigma_h$ 手裏剣、 π で平板or柱状)

D_n ($C_n + n$ 本の2回軸)

D_{nd} (D_{nh} を半分ねじる エタン、フェロセン)

以下 略で可

5 その他 S_n n は偶数 回映軸 (回転+鏡映)

クイズ

$$e^\pi > \pi^e$$

系統的分類法

参考図書: 群論の化学への応用

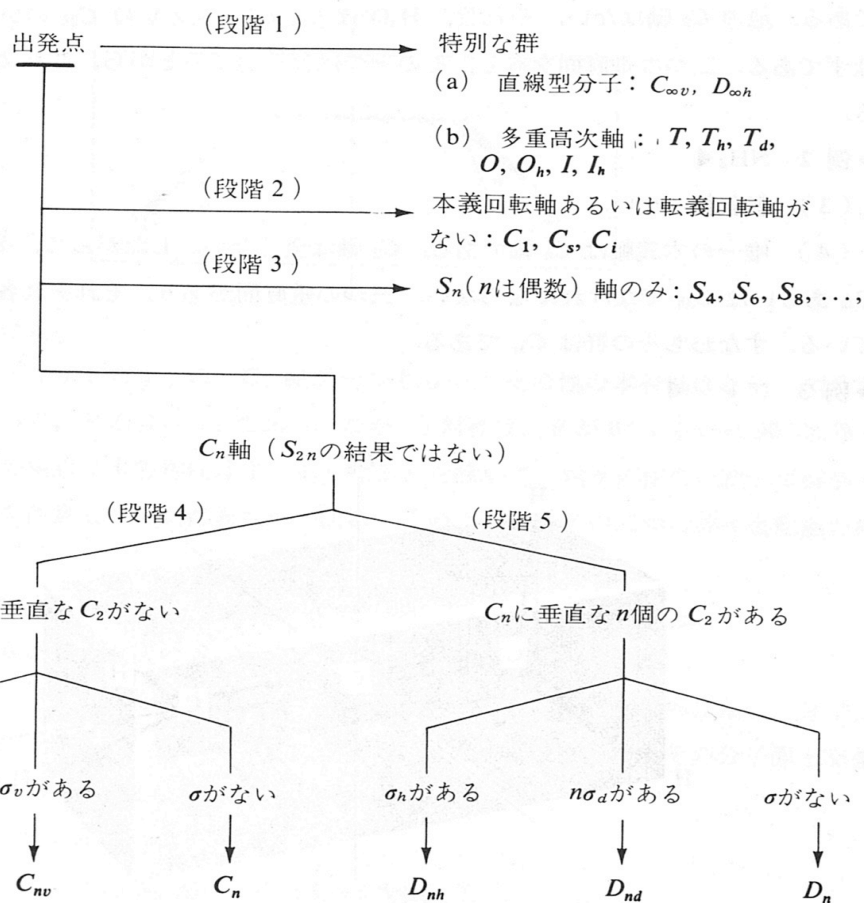
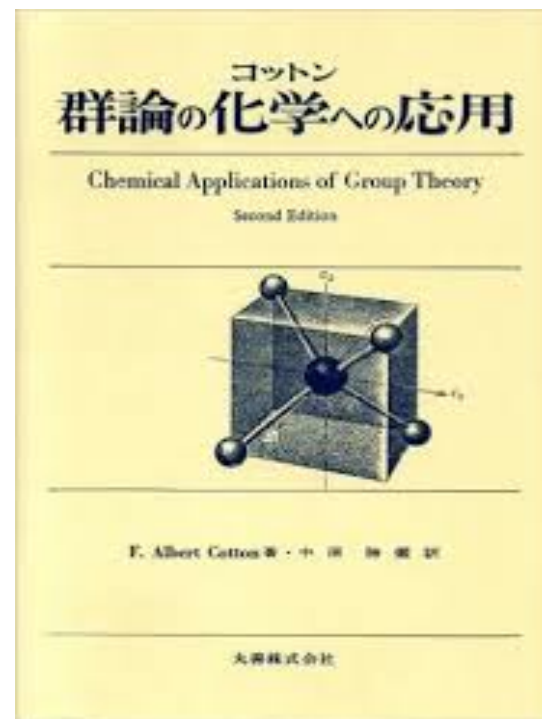


図 3.3 分子の対称性を分類するための5段階方式

第2講 表現の自由あるか？

→ 群論にはない

点群がきまると指標表からいろいろなことが分かります。

シェーンフリース記号	対称操作				並進と回転	2次の項
C_{2v}	E	C_2	$\sigma_v(xz)$	$\sigma_v(yz)$		
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	-1	-1	R_z	xy
B_1	1	-1	1	-1	x, R_y	xz
B_2	1	-1	-1	1	y, R_z	yz

表現

1次元 主軸に対して 対称A 反対称B 2次元 E 3次元 T

主軸に垂直な C_2 軸or鏡映面に対して 対称1 反対称2

対称心に対して 対称g 反対称u σ_h に対して 対称' 反対称''

付録 III

A. 化学的に重要な対称性群の指標表

(1) 非軸性群

C_1	E
A	1

C_3	E	σ_h		C_i	E	i	
A'	1	1	x, y, R_z	A_g	1	1	R_x, R_y, R_z
A''	1	-1	z, R_x, R_y	A_u	1	-1	x, y, z
			x^2, y^2, z^2, xy				x^2, y^2, z^2
			yz, xz				xy, xz, yz

(2) C_n 群

C_2	E	C_2	
A	1	1	z, R_z
B	1	-1	x, y, R_x, R_y
			x^2, y^2, z^2, xy
			yz, xz

C_3	E	C_3	C_3^2		$\varepsilon = \exp(2\pi i/3)$
A	1	1	1	z, R_z	$x^2 + y^2, z^2$
E	$\begin{pmatrix} 1 & \varepsilon & \varepsilon^* \\ 1 & \varepsilon^* & \varepsilon \end{pmatrix}$			$(x, y)(R_x, R_y)$	$(x^2 - y^2, xy)(yz, xz)$

C_4	E	C_4	C_2	C_4^3	
A	1	1	1	1	z, R_z
B	1	-1	1	-1	$x^2 + y^2, z^2$
E	$\begin{pmatrix} 1 & i & -1 & -i \\ 1 & -i & -1 & i \end{pmatrix}$				$x^2 - y^2, xy$
					$(x, y)(R_x, R_y)$
					(yz, xz)

C_5	E	C_5	C_5^2	C_5^3	C_5^4		$\varepsilon = \exp(2\pi i/5)$
A	1	1	1	1	1	z, R_z	$x^2 + y^2, z^2$
E_1	$\begin{pmatrix} 1 & \varepsilon & \varepsilon^2 & \varepsilon^{2*} & \varepsilon^* \\ 1 & \varepsilon^* & \varepsilon^{2*} & \varepsilon^2 & \varepsilon \end{pmatrix}$					$(x, y)(R_x, R_y)$	(yz, xz)
E_2	$\begin{pmatrix} 1 & \varepsilon^2 & \varepsilon^* & \varepsilon & \varepsilon^{2*} \\ 1 & \varepsilon^{2*} & \varepsilon & \varepsilon^* & \varepsilon^2 \end{pmatrix}$						$(x^2 - y^2, xy)$

C_6	E	C_6	C_3	C_2	C_3^2	C_6^5		$\varepsilon = \exp(2\pi i/6)$
A	1	1	1	1	1	1	z, R_z	$x^2 + y^2, z^2$
B	1	-1	1	-1	1	-1		
E_1	$\begin{pmatrix} 1 & \varepsilon & -\varepsilon^* & -1 & -\varepsilon & \varepsilon^* \\ 1 & \varepsilon^* & -\varepsilon & -1 & -\varepsilon^* & \varepsilon \end{pmatrix}$						(x, y)	(xz, yz)
E_2	$\begin{pmatrix} 1 & -\varepsilon^* & -\varepsilon & 1 & -\varepsilon^* & -\varepsilon \\ 1 & -\varepsilon & -\varepsilon^* & 1 & -\varepsilon & -\varepsilon^* \end{pmatrix}$						(R_x, R_y)	$(x^2 - y^2, xy)$

C_7	E	C_7	C_7^2	C_7^3	C_7^4	C_7^5	C_7^6		$\varepsilon = \exp(2\pi i/7)$
A	1	1	1	1	1	1	1	z, R_z	$x^2 + y^2, z^2$
E_1	$\begin{pmatrix} 1 & \varepsilon & \varepsilon^2 & \varepsilon^3 & \varepsilon^{3*} & \varepsilon^{2*} & \varepsilon^* \\ 1 & \varepsilon^* & \varepsilon^{2*} & \varepsilon^{3*} & \varepsilon^3 & \varepsilon^2 & \varepsilon \end{pmatrix}$							(x, y)	(xz, yz)
E_2	$\begin{pmatrix} 1 & \varepsilon^2 & \varepsilon^{3*} & \varepsilon^* & \varepsilon & \varepsilon^3 & \varepsilon^{2*} \\ 1 & \varepsilon^{2*} & \varepsilon^3 & \varepsilon & \varepsilon^* & \varepsilon^{3*} & \varepsilon^2 \end{pmatrix}$							(R_x, R_y)	$(x^2 - y^2, xy)$
E_3	$\begin{pmatrix} 1 & \varepsilon^3 & \varepsilon^* & \varepsilon^2 & \varepsilon^{2*} & \varepsilon & \varepsilon^{3*} \\ 1 & \varepsilon^{3*} & \varepsilon & \varepsilon^{2*} & \varepsilon^2 & \varepsilon^* & \varepsilon^3 \end{pmatrix}$								

C_8	E	C_8	C_4	C_2	C_4^3	C_8^3	C_8^5	C_8^7		$\varepsilon = \exp(2\pi i/8)$
A	1	1	1	1	1	1	1	1	z, R_z	$x^2 + y^2, z^2$
B	1	-1	1	1	-1	-1	-1	-1		
E_1	$\begin{pmatrix} 1 & \varepsilon & i & -1 & -i & -\varepsilon^* & -\varepsilon & \varepsilon^* \\ 1 & \varepsilon^* & -i & -1 & i & -\varepsilon & -\varepsilon^* & \varepsilon \end{pmatrix}$								(x, y)	(xz, yz)
E_2	$\begin{pmatrix} 1 & i & -1 & 1 & -1 & -i & i & -i \\ 1 & -i & -1 & 1 & -1 & i & -i & i \end{pmatrix}$								(R_x, R_y)	$(x^2 - y^2, xy)$
E_3	$\begin{pmatrix} 1 & -\varepsilon & i & -1 & -i & \varepsilon^* & \varepsilon & -\varepsilon^* \\ 1 & -\varepsilon^* & -i & -1 & i & \varepsilon & \varepsilon^* & -\varepsilon \end{pmatrix}$									

(3) D_n 群

D_2	E	$C_2(z)$	$C_2(y)$	$C_2(x)$	
A	1	1	1	1	x^2, y^2, z^2
B_1	1	1	-1	-1	z, R_z
B_2	1	-1	1	-1	xy
B_3	1	-1	-1	1	y, R_y
					xz
					x, R_x
					yz

D_3	E	$2C_3$	$3C_2$		
A_1	1	1	1		$x^2 + y^2, z^2$
A_2	1	1	-1	z, R_z	
E	2	-1	0	$(x, y)(R_x, R_y)$	$(x^2 - y^2, xy)(xz, yz)$

D_4	E	$2C_4$	$C_2(=C_4^2)$	$2C_2'$	$2C_2''$		
A_1	1	1	1	1	1	z, R_z	$x^2 + y^2, z^2$
A_2	1	1	1	-1	-1		
B_1	1	-1	1	1	-1		$x^2 - y^2$
B_2	1	-1	1	-1	1		xy
E	2	0	-2	0	0	$(x, y)(R_x, R_y)$	(xz, yz)

D_5	E	$2C_5$	$2C_5^2$	$5C_2$		
A_1	1	1	1	1	z, R_z	$x^2 + y^2, z^2$
A_2	1	1	1	-1		
E_1	2	$2 \cos 72^\circ$	$2 \cos 144^\circ$	0	$(x, y)(R_x, R_y)$	(xz, yz)
E_2	2	$2 \cos 144^\circ$	$2 \cos 72^\circ$	0		$(x^2 - y^2, xy)$

D_6	E	$2C_6$	$2C_3$	C_2	$3C_2'$	$3C_2''$		
A_1	1	1	1	1	1	1	z, R_z	$x^2 + y^2, z^2$
A_2	1	1	1	1	-1	-1		
B_1	1	-1	1	-1	1	-1		
B_2	1	-1	1	-1	-1	1		
E_1	2	1	-1	-2	0	0	$(x, y)(R_x, R_y)$	(xz, yz)
E_2	2	-1	-1	2	0	0		$(x^2 - y^2, xy)$

(4) C_{nv} 群

C_{2v}	E	C_2	$\sigma_v(xz)$	$\sigma_v'(yz)$		
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	-1	-1	R_z	xy
B_1	1	-1	1	-1	x, R_y	xz
B_2	1	-1	-1	1	y, R_x	yz

C_{3v}	E	$2C_3$	$3\sigma_v$		
A_1	1	1	1	z	$x^2 + y^2, z^2$
A_2	1	1	-1	R_z	
E	2	-1	0	$(x, y)(R_x, R_y)$	$(x^2 - y^2, xy)(xz, yz)$

C_{4v}	E	$2C_4$	C_2	$2\sigma_v$	$2\sigma_d$		
A_1	1	1	1	1	1	z	$x^2 + y^2, z^2$
A_2	1	1	1	-1	-1	R_z	
B_1	1	-1	1	1	-1		$x^2 - y^2$
B_2	1	-1	1	-1	1		xy
E	2	0	-2	0	0	$(x, y)(R_x, R_y)$	(xz, yz)

C_{5v}	E	$2C_5$	$2C_5^2$	$5\sigma_v$		
A_1	1	1	1	1	z	$x^2 + y^2, z^2$
A_2	1	1	1	-1	R_z	
E_1	2	$2 \cos 72^\circ$	$2 \cos 144^\circ$	0	$(x, y)(R_x, R_y)$	(xz, yz)
E_2	2	$2 \cos 144^\circ$	$2 \cos 72^\circ$	0		$(x^2 - y^2, xy)$

C_{6v}	E	$2C_6$	$2C_3$	C_2	$3\sigma_v$	$3\sigma_d$		
A_1	1	1	1	1	1	1	z	$x^2 + y^2, z^2$
A_2	1	1	1	1	-1	-1	R_z	
B_1	1	-1	1	-1	1	-1		
B_2	1	-1	1	-1	-1	1		
E_1	2	1	-1	-2	0	0	$(x, y)(R_x, R_y)$	(xz, yz)
E_2	2	-1	-1	2	0	0		$(x^2 - y^2, xy)$

(5) C_{nh} 群

C_{2h}	E	C_2	i	σ_h		
A_g	1	1	1	1	R_z	x^2, y^2, z^2, xy
B_g	1	-1	1	-1	R_x, R_y	xz, yz
A_u	1	1	-1	-1	z	
B_u	1	-1	-1	1	x, y	

C_{3h}	E	C_3	C_3^2	σ_h	S_3	S_3^5		$\varepsilon = \exp(2\pi i/3)$
A'	1	1	1	1	1	1	R_z	$x^2 + y^2, z^2$
E'	$\begin{Bmatrix} 1 & \varepsilon & \varepsilon^* \\ 1 & \varepsilon^* & \varepsilon \end{Bmatrix}$	ε	ε^*	1	ε	ε^*	(x, y)	$(x^2 - y^2, xy)$
A''	1	1	1	-1	-1	-1	z	
E''	$\begin{Bmatrix} 1 & \varepsilon & \varepsilon^* \\ 1 & \varepsilon^* & \varepsilon \end{Bmatrix}$	ε	ε^*	-1	$-\varepsilon$	$-\varepsilon^*$	(R_x, R_y)	(xz, yz)

C_{4h}	E	C_4	C_2	C_4^3	i	S_4^3	σ_h	S_4		
A_g	1	1	1	1	1	1	1	1	R_z	$x^2 + y^2, z^2$
B_g	1	-1	1	-1	1	-1	1	-1		$x^2 - y^2, xy$
E_g	1	i	-1	$-i$	1	i	-1	$-i$	(R_x, R_y)	(xz, yz)
A_u	1	1	1	1	1	1	1	1		z
B_u	1	-1	1	-1	1	-1	1	-1	(x, y)	
E_u	1	i	-1	$-i$	1	i	-1	$-i$		

C_{5h}	E	C_5	C_5^2	C_5^3	C_5^4	σ_h	S_5	S_5^7	S_5^3	S_5^9		$\varepsilon = \exp(2\pi i/5)$
A'	1	1	1	1	1	1	1	1	1	1	R_z	$x^2 + y^2, z^2$
E_1'	1	ε	ε^2	ε^2*	$\varepsilon*$	1	ε	ε^2	ε^2*	$\varepsilon*$		(x, y)
E_2'	1	ε^2	$\varepsilon*$	ε	ε^2*	1	ε^2	$\varepsilon*$	ε	ε^2*	z	$(x^2 - y^2, xy)$
A''	1	1	1	1	1	1	1	1	1	1		(R_x, R_y)
E_1''	1	ε	ε^2	ε^2*	$\varepsilon*$	-1	ε	ε^2	ε^2*	$\varepsilon*$	(x, y)	
E_2''	1	ε^2	$\varepsilon*$	ε	ε^2*	-1	ε^2	$\varepsilon*$	ε	ε^2*		

C_{6h}	E	C_6	C_3	C_2	C_3^2	C_6^5	i	S_3^5	S_6^5	σ_h	S_6	S_3		$\varepsilon = \exp(2\pi i/6)$
A_g	1	1	1	1	1	1	1	1	1	1	1	1	R_z	$x^2 + y^2, z^2$
B_g	1	-1	1	-1	1	-1	1	-1	1	-1	1	-1		(R_x, R_y)
E_{1g}	1	ε	ε^2	ε^2*	$\varepsilon*$	1	ε	ε^2	ε^2*	$\varepsilon*$	1	ε	(x, y)	
E_{2g}	1	ε^2	$\varepsilon*$	ε	ε^2*	1	ε^2	$\varepsilon*$	ε	ε^2*	1	ε^2		(R_x, R_y)
A_u	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1	z	
B_u	1	-1	1	-1	1	-1	-1	1	-1	1	-1	1		(x, y)
E_{1u}	1	ε	ε^2	ε^2*	$\varepsilon*$	-1	ε	ε^2	ε^2*	$\varepsilon*$	-1	ε	(x, y)	
E_{2u}	1	ε^2	$\varepsilon*$	ε	ε^2*	-1	ε^2	$\varepsilon*$	ε	ε^2*	-1	ε^2		

(6) D_{nh} 群

D_{2h}	E	$C_2(z)$	$C_2(y)$	$C_2(x)$	i	$\sigma(xy)$	$\sigma(xz)$	$\sigma(yz)$		
A_g	1	1	1	1	1	1	1	1	R_z	x^2, y^2, z^2
B_{1g}	1	1	-1	-1	1	1	-1	-1		xy
B_{2g}	1	-1	1	-1	1	-1	1	-1	xz	
B_{3g}	1	-1	-1	1	1	-1	-1	1	yz	
A_u	1	1	1	1	1	-1	-1	-1	R_x	
B_{1u}	1	1	-1	-1	1	-1	1	-1		z
B_{2u}	1	-1	1	-1	1	1	-1	1	y	
B_{3u}	1	-1	-1	1	1	1	-1	-1	x	

D_{3h}	E	$2C_3$	$3C_2$	σ_h	$2S_3$	$3\sigma_v$		
A_1'	1	1	1	1	1	1	R_z	$x^2 + y^2, z^2$
A_2'	1	1	-1	1	1	-1		(x, y)
E'	2	-1	0	2	-1	0	z	
A_1''	1	1	1	-1	-1	1		(R_x, R_y)
A_2''	1	1	-1	-1	-1	1		
E''	2	-1	0	-2	1	0		

D_{4h}	E	$2C_4$	C_2	$2C_2'$	$2C_2''$	i	$2S_4$	σ_h	$2\sigma_v$	$2\sigma_d$		
A_{1g}	1	1	1	1	1	1	1	1	1	1	R_z	$x^2 + y^2, z^2$
A_{2g}	1	1	1	-1	-1	1	1	1	-1	-1		$x^2 - y^2$
B_{1g}	1	-1	1	1	-1	1	-1	1	1	-1	(R_x, R_y)	xy
B_{2g}	1	-1	1	-1	1	1	-1	1	-1	1		(xz, yz)
E_g	2	0	-2	0	0	2	0	-2	0	0	z	
A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1		(x, y)
A_{2u}	1	1	1	-1	-1	-1	-1	-1	1	1		
B_{1u}	1	-1	1	1	-1	-1	1	-1	1	-1		
B_{2u}	1	-1	1	-1	1	-1	1	-1	-1	1		
E_u	2	0	-2	0	0	-2	0	2	0	0		

D_{5h}	E	$2C_5$	$2C_5^2$	$5C_2$	σ_h	$2S_5$	$2S_5^3$	$5\sigma_v$		
A_1'	1	1	1	1	1	1	1	1	R_z	$x^2 + y^2, z^2$
A_2'	1	1	1	-1	1	1	1	-1		(x, y)
E_1'	2	$2 \cos 72^\circ$	$2 \cos 144^\circ$	0	2	$2 \cos 72^\circ$	$2 \cos 144^\circ$	0	z	$(x^2 - y^2, xy)$
E_2'	2	$2 \cos 144^\circ$	$2 \cos 72^\circ$	0	2	$2 \cos 144^\circ$	$2 \cos 72^\circ$	0		(R_x, R_y)
A_1''	1	1	1	1	-1	-1	-1	-1	(x, y)	
A_2''	1	1	1	-1	-1	-1	-1	1		z
E_1''	2	$2 \cos 72^\circ$	$2 \cos 144^\circ$	0	-2	$-2 \cos 72^\circ$	$-2 \cos 144^\circ$	0	(R_x, R_y)	(xz, yz)
E_2''	2	$2 \cos 144^\circ$	$2 \cos 72^\circ$	0	-2	$-2 \cos 144^\circ$	$-2 \cos 72^\circ$	0		

D_{6h}	E	$2C_6$	$2C_3$	C_2	$3C_2'$	$3C_2''$	i	$2S_3$	$2S_6$	σ_h	$3\sigma_d$	$3\sigma_v$		
A_{1g}	1	1	1	1	1	1	1	1	1	1	1	1	R_z	$x^2 + y^2, z^2$
A_{2g}	1	1	1	1	-1	-1	1	1	1	1	-1	-1		(R_x, R_y)
B_{1g}	1	-1	1	-1	1	-1	1	-1	1	-1	1	-1	(R_x, R_y)	$(x^2 - y^2, xy)$
B_{2g}	1	-1	1	-1	-1	1	1	-1	-1	1	-1	1		z
E_{1g}	2	1	-1	-2	0	0	2	1	-1	-2	0	0	(x, y)	
E_{2g}	2	-1	1	2	0	0	2	-1	1	2	0	0		
A_{1u}	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1	z	
A_{2u}	1	1	1	1	-1	-1	-1	-1	-1	-1	1	1		(x, y)
B_{1u}	1	-1	1	-1	1	-1	-1	1	-1	1	1	-1		
B_{2u}	1	-1	1	-1	-1	1	-1	1	-1	1	-1	1		
E_{1u}	2	1	-1	-2	0	0	-2	-1	1	2	0	0		
E_{2u}	2	-1	1	2	0	0	-2	1	-1	-2	0	0		

D_{8h}	E	$2C_8$	$2C_8^3$	$2C_4$	C_2	$4C_2'$	$4C_2''$	i	$2S_8$	$2S_8^3$	$2S_4$	σ_h	$4\sigma_d$	$4\sigma_v$		
A_{1g}	1	1	1	1	1	1	1	1	1	1	1	1	1	1	R_z	$x^2 + y^2, z^2$
A_{2g}	1	1	1	1	1	-1	-1	1	1	1	1	1	-1	-1		(R_x, R_y)
B_{1g}	1	-1	-1	1	1	1	-1	1	-1	-1	1	1	1	-1	(R_x, R_y)	$(x^2 - y^2, xy)$
B_{2g}	1	-1	-1	1	1	-1	1	1	-1	-1	1	1	-1	1		z
E_{1g}	2	$\sqrt{2}$	$-\sqrt{2}$	0	-2	0	0	2	$\sqrt{2}$	$-\sqrt{2}$	0	-2	0	0	(x, y)	
E_{2g}	2	0	0	-2	2	0	0	2	0	0	-2	0	0			
E_{3g}	2	$-\sqrt{2}$	$\sqrt{2}$	0	-2	0	0	-2	$-\sqrt{2}$	$\sqrt{2}$	0	-2	0	0		
A_{1u}	1	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1	-1	z	
A_{2u}	1	1	1	1	1	-1	-1	-1	-1	-1	-1	-1	1	1		(x, y)
B_{1u}	1	-1	-1	1	1	1	-1	-1	1	1	1	-1	-1	-1		
B_{2u}	1	-1	-1	1	1	-1	-1	-1	1	1	1	-1	-1	1		
E_{1u}	2	$\sqrt{2}$	$-\sqrt{2}$	0	-2	0	0	-2	$-\sqrt{2}$	$\sqrt{2}$	0	2	0	0		
E_{2u}	2	0	0	-2	2	0	0	-2	0	0	2	-2	0	0		
E_{3u}	2	$-\sqrt{2}$	$\sqrt{2}$	0	-2	0	0	-2	$\sqrt{2}$	$-\sqrt{2}$	0	2	0	0		